

GPT

GPT-one-hot

drfp RBF

one-hot Tanimoto

drfp linear

rxnfp linear

rxnfp RBF

accuracy

0.4

0.2

F₁ macro

0.4

0.2

F₁ micro

0.4

0.2

0.0

25

50

75

100

125

150

175

200

